Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 8.38

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 4.48e-01

Nearest Neighbors from the Training Set

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4-Hydroxybenzoic acid	Salicylic acid	1-Hexadecanol
Measured: 8.08	**Measured:** 7.44	**Measured:** 9.90
Predicted: 7.78	**Predicted:** 7.60	**Predicted:** 9.79

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Diphenylamine	1-Octadecanol
Measured: 7.64	**Measured:** 10.9
Predicted: 8.73	**Predicted:** 10.5